Radiation Physics Note 80

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OBSERVATIONS ON SPECTRUM UNFOLDING WITH BUNKI

INTRODUCTION

Spectrum unfolding, as has been discussed by many authors,[1] has inherent difficulties that effect the reliability of the results. These problems arise from the mathematically underdetermined and sometimes ill-conditioned nature of the procedures.

The underdetermined nature (eight equations in thirty-one unknowns) manifests itself as more than one solution spectrum that describe the data equally well. While a priori information can be used to eliminate solutions that give negative fluxes or those that lead to neutron energies above that of the accelerator, many other solution sets may still exist.

The MAXIET algorithm in the BUNKI iterative recursion unfolding program[2] represents an attempt to obtain a physically reasonable spectrum by specifying the shape of the initial solution as having a high energy peak, a slowing-down (1/E-type) term, and a thermal component. This is consistent with what is expected for neutrons produced through scattering, moderation, and absorption around particle accelerators. To reduce any fluctuations and oscillations in solutions, smoothing to the initial spectral shape can also be requested. MAXIET alone, without the use of the rest of BUNKI to unfold the spectrum, completely overcomes the underdeterminate nature of the problem by constraining the spectral shape to a functional form having only four parameters.

The ill-conditioned nature of the spectrum unfolding problem implies that small uncertainties in the actual sphere response data or similarities in the detector response functions for two or more detectors may translate into large uncertainties in the unfolded spectrum. Statistical, as well as systematic, errors in measured sphere responses can sometimes lead to substantial differences in spectral shape.

TEST SPECTRA

Single and multiple group test spectra can be generated, as discussed by Couch[3] (in connection with studies using the unfolding code SWIFT), by use of "known" response matrices. Fig. 1 shows the result of unfolding, with SPUNIT in the BUNKI program, single and double group spectra created from the 4 mm by 4 mm ^{6}LiI detector response matrix of Sanna.[4] The results are the same whether the MAXIET prescription or a 1/E shape is used as the initial solution to unfolding with 1000 iterations. Fig. 2 shows a more complex, triple-group, spectrum unfolded (1000 iterations) with both 1/E and MAXIET initial solutions. The sphere responses were constructed for unit neutron fluence in energy bins 1, 20, and 25. Although the fit to sphere responses is good in both cases, the unfolded spectral shapes reflect a dependence on initial conditions. Note that the MAXIET algorithm constrains the solution to a single high energy peak in the neutron spectrum; in this case a best fit is obtained for a single peak at an energy of 2 to 3 MeV, a value between the mean energies of bins 20 and 25. Starting with this initial solution, 1000 iterations with SPUNIT resulted in an unfolded spectrum with two fairly narrow high energy peaks (plus a thermal peak), each with a total fluence of about unity, in agreement with the way the sphere responses were initially constructed.

Fig. 3 shows the spectrum unfolded from sphere responses constructed to correspond to a distribution with unit neutron fluence in each of the thirty-one energy bins. Note that fluence, and <u>not</u> fluence per unit lethargy, is plotted as the ordinate in this figure. As seen, the unfolded fluence is unity to ±15% over all energies except the lowest two bins, although the spectrum displays fluctuations around this value.

Fig. 4 shows the results of unfolding sphere responses for a three group spectrum (i.e., unit fluence in bins 1, 20, and 25) with the original responses perturbed according to a normal distribution with a sigma of 1% and 10%. This tests the stability of the unfolded spectrum to statistical uncertainties in sphere responses, and thus checks for ill-conditioned solutions. At the 10% level, the shape of the unfolded spectrum starts to deviate from that based on unperturbed responses, although the general properties of the two spectra are not too dissimilar.

ACTUAL DATA

Fig. 5 shows spectra unfolded under various conditions for actual sphere responses determined by use of TLD 600, 700 detectors in AP50 during some shielding studies conducted by E760. The results indicate clearly that the shape of the unfolded spectrum can depend on the initial conditions. Smoothing tends to make the final spectrum look more like the initial one. Note that the error between calculated and measured sphere responses, when the solution is constrained to that given by the MAXIET algorithm (i.e., 0 iterations), is almost as good as the final fit after 20000 iterations. This suggests that the data does reflect the MAXIET spectral shape, and as such the solution represents a mathematically well behaved result. The slightly better fit obtained by allowing more and more iterations arises at the expense of adding nonphysical oscillations into the final spectrum. Smoothing the final result (for 10000 iterations) decreases the goodness of fit to almost the value for no iterations! To the extent that a satisfactory fit to measured sphere responses is obtained by use of the MAXIET algorithm, no further iterative fitting is needed.

As seen in Fig. 5, spectra unfolded by starting with an 1/E initial solution, have a larger high-energy neutron component than those constrained by the MAXIET subroutine. This leads to somewhat larger values of absorbed dose and smaller quality factors, as seen in Table 1. Note also that values of the entities shown (which are broad integrals of the unfolded spectrum convoluted with other functions) are quite dependent on the number of iterations for spectra based on 1/E starting solutions, although goodness of fit is about the same in both cases. This dependence apparently arises from "spurious" structure introduced through excessive and needless iteration.

Fig. 6 compares the spectrum unfolded from unperturbed AP50 sphere responses with that from responses displaced from these according to a normal distribution with a sigma of 10%. The observed spectral differences reflect the effects of a 10% statistical uncertainty on each sphere response, and imply that the solution is somewhat ill-conditioned at this level of accuracy.

To gain confidence in the validity of the unfolded spectrum it is useful to use more than one unfolding method. Fig. 7 compares AP50 spectra unfolded by both BUNKI and the constrained least squares code LOUHI.[5] In both cases the initial spectrum was chosen to have an 1/E dependence, and the final spectrum was smoothed to the initial shape. Both methods reveal a thermal peak and one at an energy near 1 MeV, and predict similar values of dose, dose-equivalent, and quality factor. Otherwise, however, agreement in detail is poor.

CONCLUSION

It is not possible to completely specify a generic procedure for unfolding Bonner Sphere response data. The following are some questions to ask and some points to keep in mind.

1. Does the MAXIET solution alone (no iterations) give reasonable fits to the measured sphere responses? Investigate the fits starting with different values of T and delta-T (i.e., high energy peak energy and perturbation step size).

2. If MAXIET fits are poor, perform only as many iterations as necessary to get a reasonable fit. An excess number of iterations tend to generate spurious structure or oscillation in the unfolded spectrum. Are similar results obtained with both 1/E and MAXIET starting solutions?

3. Try the minimum amount of smoothing that preserves the goodness of fit, but reduces oscillations, particularly those only 1 or 2 energy bins wide.

4. Is there really a high energy neutron peak? Refit the data without the 18 inch sphere.

5. To obtain further confidence in the "final" result, use at least one other unfolding code (LOUHI, SWIFT, etc.).

Finally, the existence of high energy (>10-15 MeV) neutrons in the enclosures and outside of shielding around the TEVATRON and in the Fermilab experimental areas has been and continues to be of interest for both operational and theoretical health physics reasons. Thus, a primary concern in any unfolding analysis must be the validity of any perceived high energy peaks based on the use of Bonner Spheres.

At the same time, from an experimental point of view the Safety Section should work to develop a neutron detector for energies >10 MeV that is more sensitive/efficient than the 18 inch sphere. Techniques based on ^{11}C activation analysis and the use of NE-213 liquid scintillators are well-known elsewhere, and in the near term should be used here. Over the long-term a program emphasizing new techniques (e.g., possibly the use of BGO) would be exciting.

REFERENCES

1. For a list of references, see: J.D. Cossairt, J.G. Couch, A.J. Elwyn, and W.S. Freeman, "Radiation Measurements in a Labyrinth Penetration at a High-Energy Accelerator," Health Phys. 49, 907 (1985).

2. K.A. Lowry and T.L. Johnson, Modifications to Iterative Recursion Unfolding Algorithms and Computer Codes to Find More Appropriate Neutron Spectra, Naval Research Lab, Washington, D.C., NRL Memo Rep. 5340 (1984).

3. Jack Couch, Test Spectra for Testing Neutron Spectrum Unfolding Programs, Fermilab Radiation Physics Note 45 (Aug. 1984).

4. R.S. Sanna, Thirty-One Group Response Matrices for the Multisphere Neutron Spectrometer Over the Energy Range Thermal to 400 MeV, USAEC Report HASL-267 (1973).

5. J.T. Routti, "Interactive Graphical Computing for Simulating and Unfolding Measured Distributions," Comput. Phys. Commun. 4, 33 (1972); J.T. Routti and J.V. Sandberg "General Purpose Unfolding Program LOUHI 78 with Linear and Nonlinear Regularizations," Comput. Phys. Common. 21, 119 (1980).

FIGURES

1. Unfolded single group lethargy spectra (Top and Middle). Unfolded double group spectrum (Bottom).

2. Unfolded triple group lethargy spectra for bins 1, 20, and 25 based on MAXIET (Top) and 1/E initial conditions (Bottom). The numbers in parenthesis reflect the percent error in the fit to sphere responses.

3. Unfolded <u>fluence</u> spectrum from sphere responses constructed to correspond to unit neutron fluence in each of the thirty-one energy bins. The unfolded fluence spectrum has 1 ± 0.15 neutrons cm^{-2} in each bin except bin 1 (1.35 $n\text{-}cm^{-2}$) and bin 2 (0.45 $n\text{-}cm^{-2}$). The spectrum was unfolded starting with an 1/E shape.

4. Comparison of spectra unfolded from unperturbed sphere responses, and from responses perturbed assuming 1% errors and 10% errors, respectively.

5. Unfolded spectra based on 1/E starting values (Left) and MAXIET initial conditions (Right) for various maximum iterations. The percentage errors in the fit to sphere responses are shown for each situation.

6. Comparison of the spectrum unfolded from unperturbed sphere responses (Left) with that from responses perturbed by 10% (Right) for different number of iterations in the unfolding. The fit to the sphere responses is shown as the percentage errors on the figures.

7. Comparison of the AP50 spectrum unfolded with BUNKI with that unfolded using LOUHI.

TABLE 1

Properties of Spectra Shown in Fig. 5

Start	Iterations	Fluence (n/cm^2)	Dose (E-03 mrad)	D.E. (E-03 mrem)	Q.F.	Error (%)
MAXIET	0	824.6	1.01	6.37	6.3	3.7
	1000	833.2	1.02	6.37	6.23	3
	10000	833.2	1.05	6.54	6.22	2.8
	10000 (.01 smooth)	834.1	1.01	6.25	6.19	3.1
	20000	837.6	1.09	6.66	6.12	2.8
1/E	1	822.9	1.75	8.64	4.95	17.4
	1000	856.2	1.4	7.87	5.65	2.9
	10000	881	1.88	9.5	5.06	2.7
	10000 (.01 smooth)	846.2	1.2	7.16	5.96	3
	20000	889	2.06	10	4.87	2.7

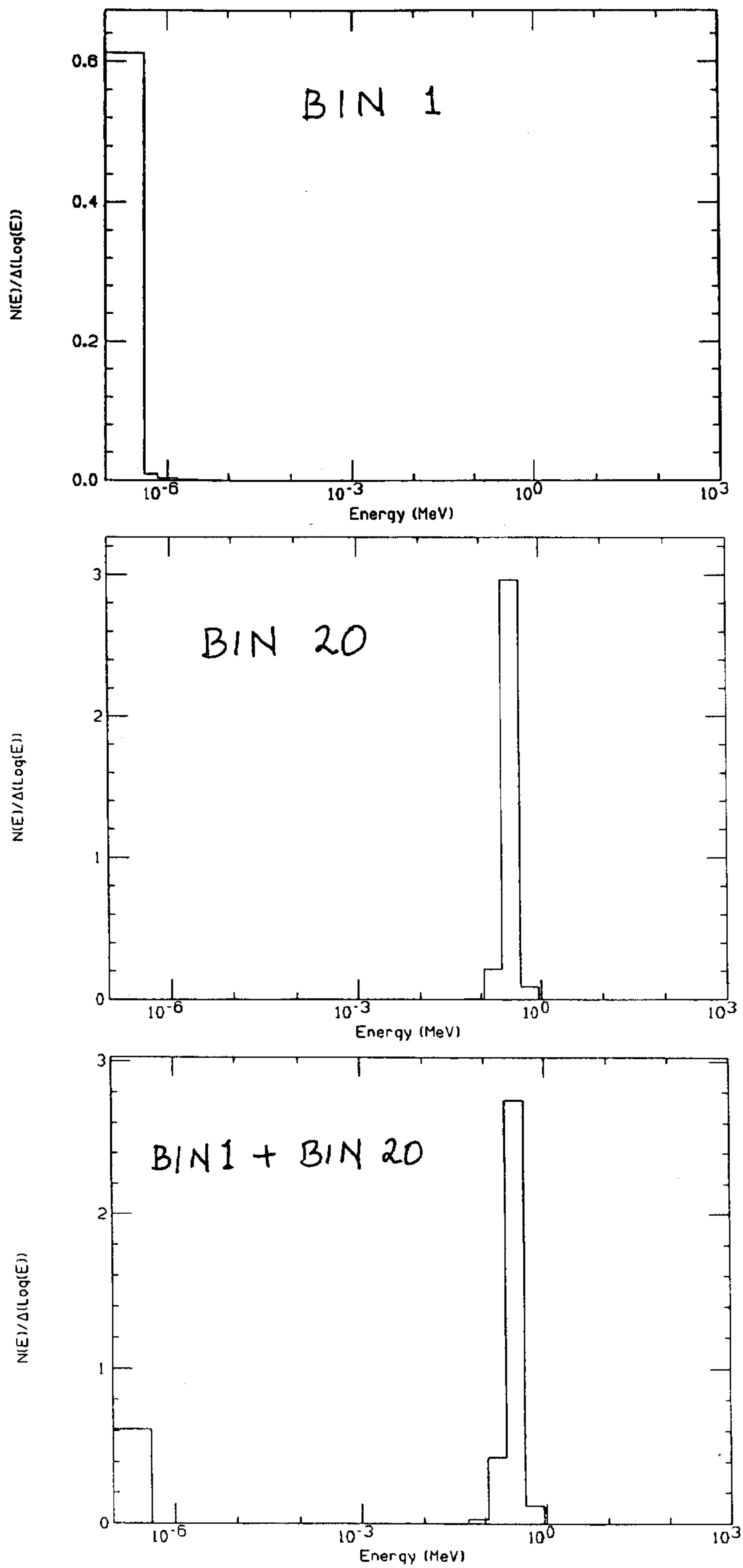

BIN 1
N(E)/Δ(Log(E))
0.0
0.2
0.4
0.6
10-6
10-3
100
103
Energy (MeV)
BIN 20
N(E)/Δ(Log(E))
0
1
2
3
10-6
10-3
100
103
Energy (MeV)
BIN1 + BIN 20
N(E)/Δ(Log(E))
0
1
2
3
10-6
10-3
100
103
Energy (MeV)

Fig. 1

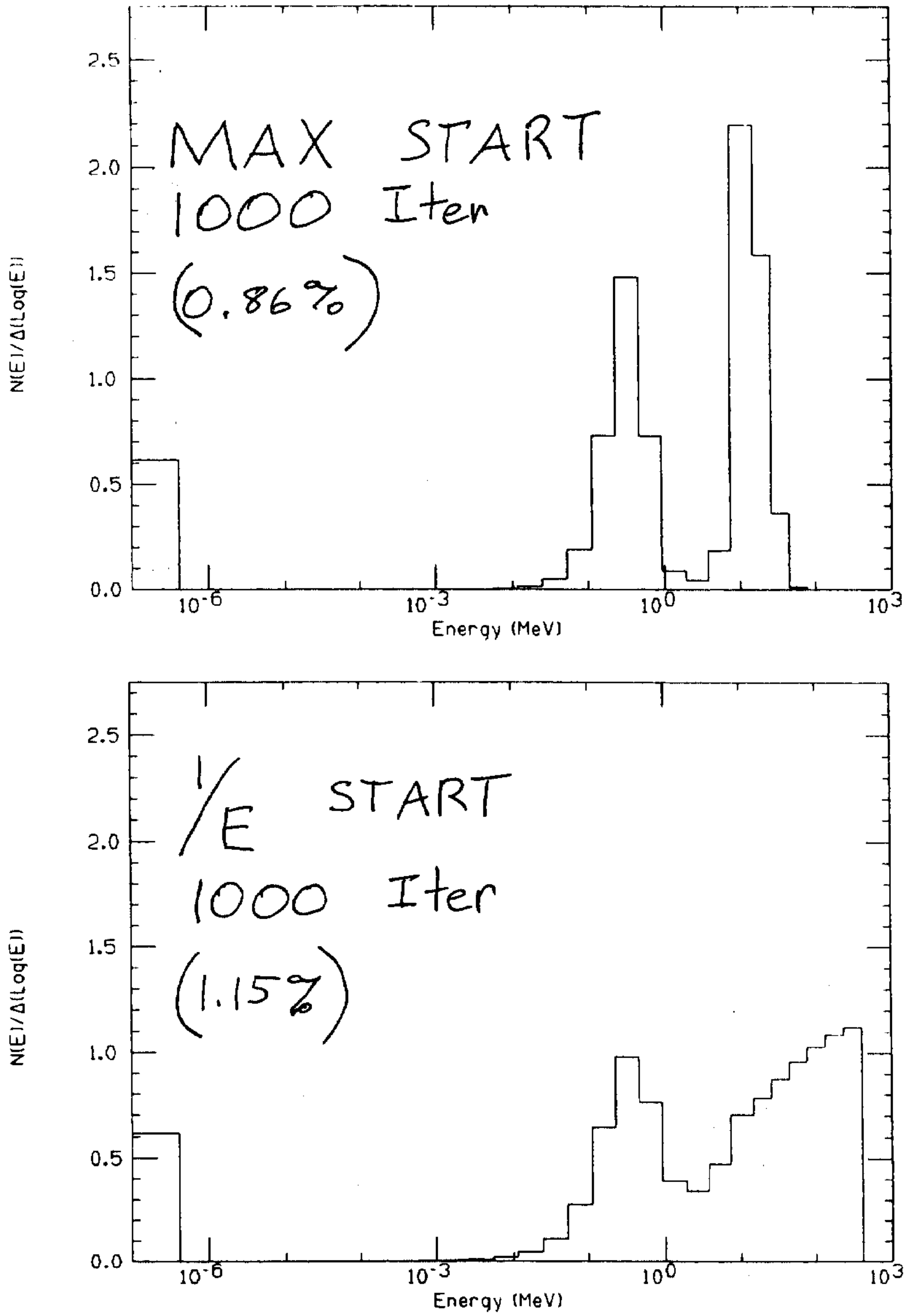

MAX START
1000 Iter
(0.86%)
N(E)/Δ(Log(E))
2.5
2.0
1.5
1.0
0.5
0.0
10^{-6}
10^{-3}
10^{0}
10^{3}
Energy (MeV)
1/E START
1000 Iter
(1.15%)
N(E)/Δ(Log(E))
2.5
2.0
1.5
1.0
0.5
0.0
10^{-6}
10^{-3}
10^{0}
10^{3}
Energy (MeV)

Fig. 2

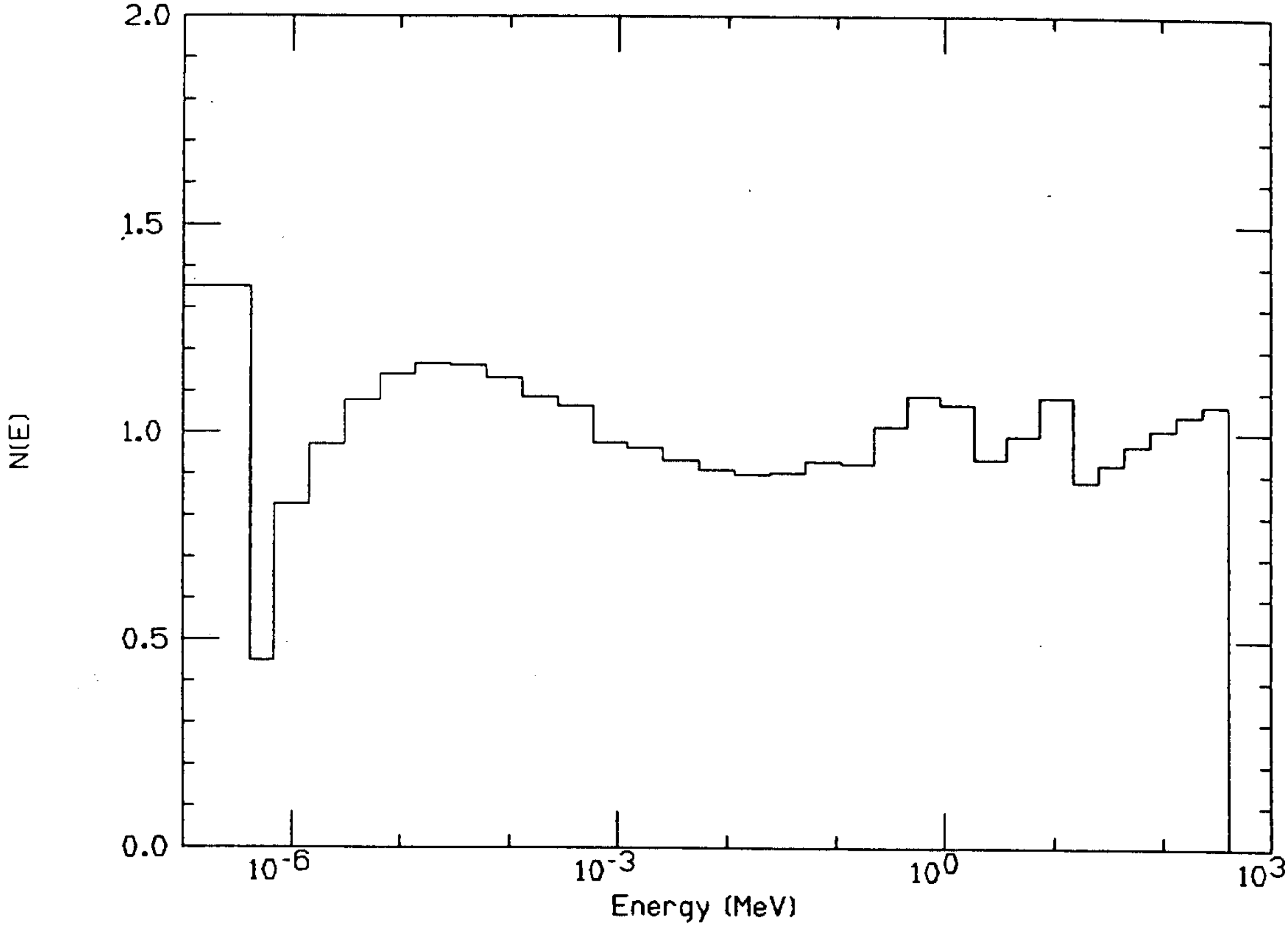


Fig. 3

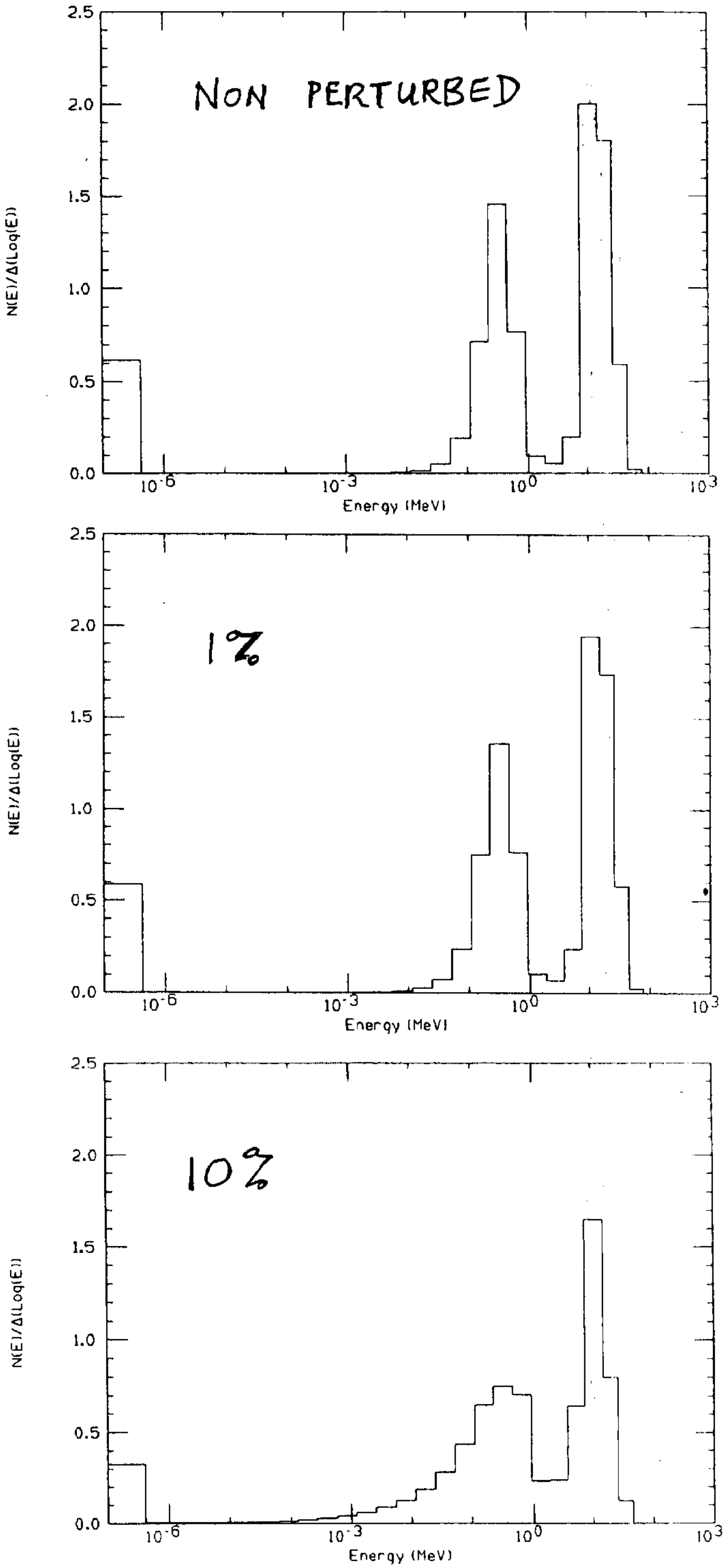

NON PERTURBED
1%
10%
N(E)/Δ(Log(E))
Energy (MeV)
0.0
0.5
1.0
1.5
2.0
2.5
10^{-6}
10^{-3}
10^{0}
10^{3}

Fig. 4

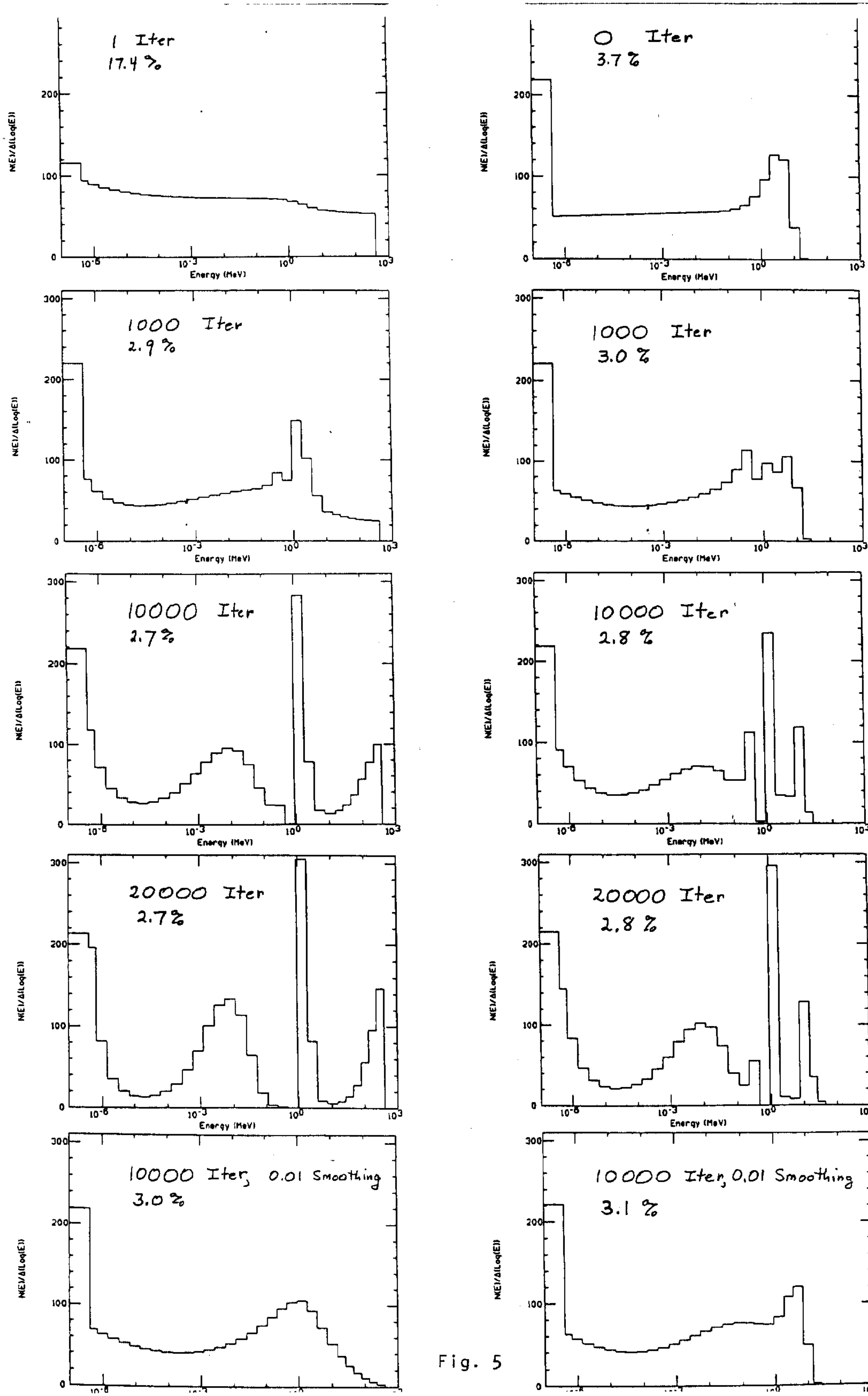
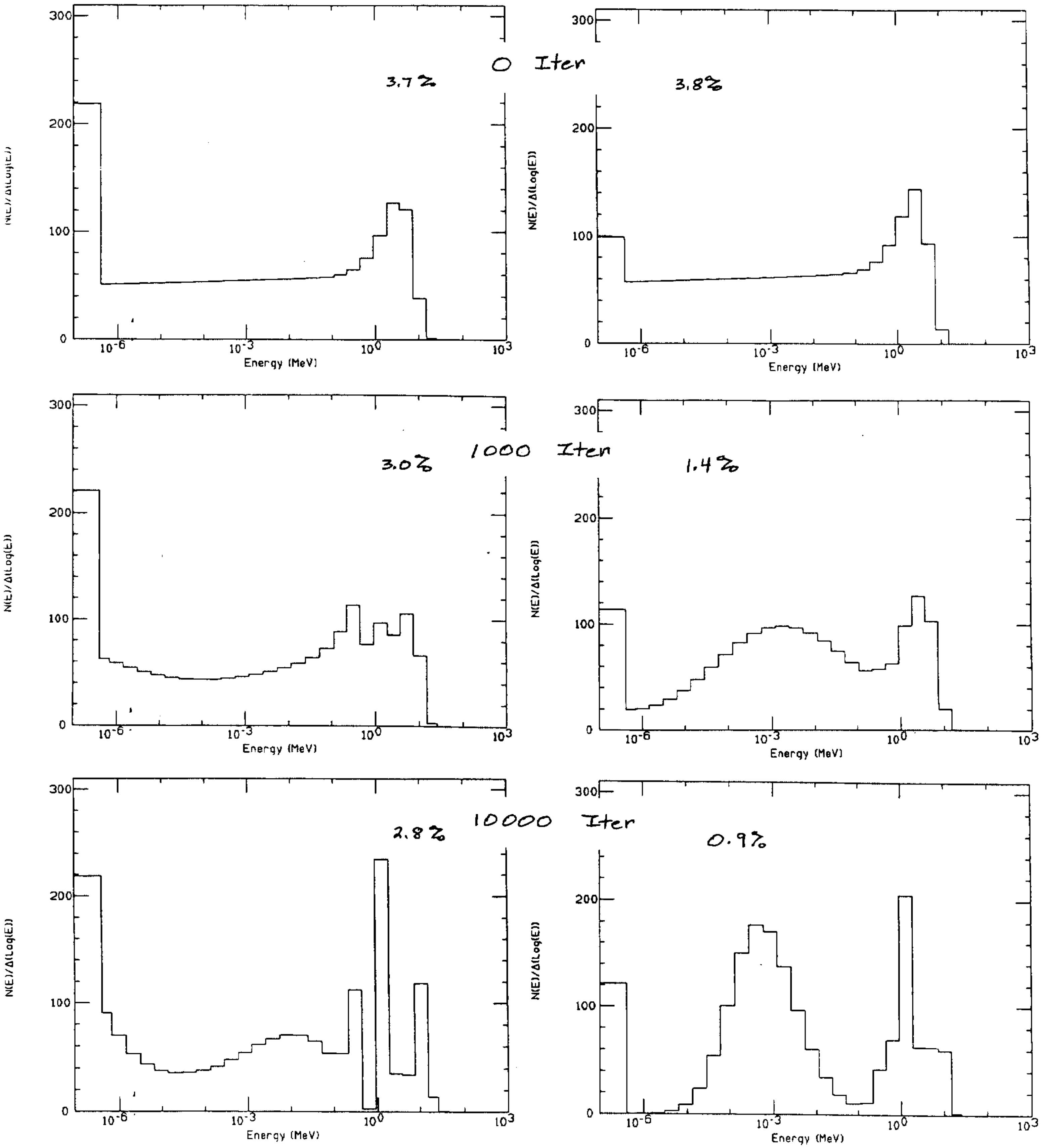
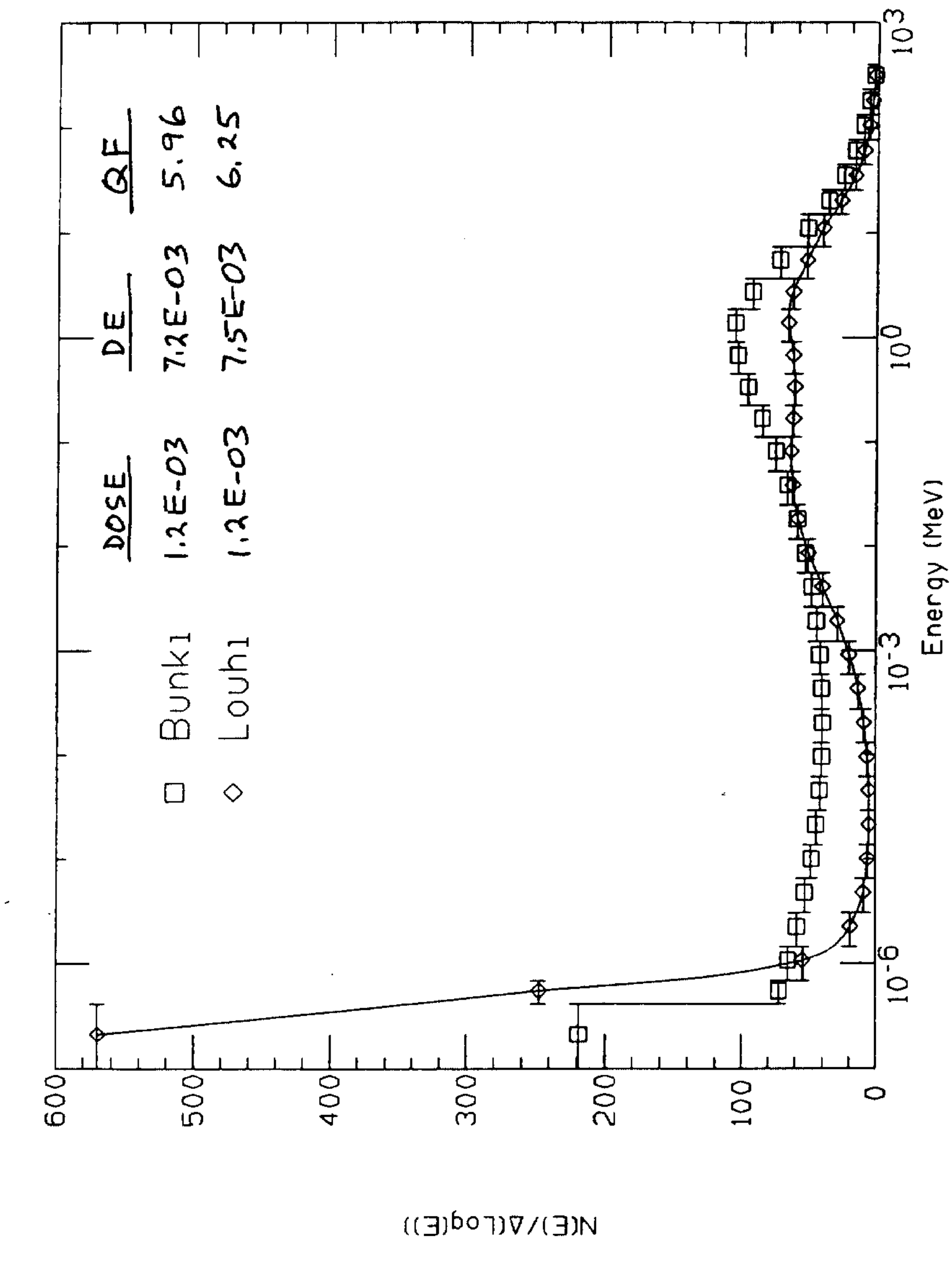

1 Iter
17.4 %
0 Iter
3.7 %
1000 Iter
2.9 %
1000 Iter
3.0 %
10000 Iter
2.7 %
10000 Iter
2.8 %
20000 Iter
2.7 %
20000 Iter
2.8 %
10000 Iter, 0.01 Smoothing
3.0 %
10000 Iter, 0.01 Smoothing
3.1 %
N(E)/Δ(Log(E))
Energy (MeV)

Fig. 5



0 Iter
3.7%
3.8%
1000 Iter
3.0%
1.4%
10000 Iter
2.8%
0.9%
N(E)/Δ(Log(E))
Energy (MeV)

Fig. 6



Bunk1
Louh1
DOSE
1.2E-03
1.2E-03
DE
7.2E-03
7.5E-03
QF
5.96
6.25
Energy (MeV)
N(E)/Δ(Log(E))

Fig. 7